International Journal of Trend in Scientific Research and Development (IJTSRD)
Volume 7 Issue 3, May-June 2023 Available Online: www.ijtsrd.com e-ISSN: 2456 – 6470

Impact of Artificial Intelligence in the Pharmaceutical World- A Review

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ABSTRACT

The pharmaceutical industry stands to be transformed by Artificial Intelligence (AI), particularly in areas such as drug discovery, clinical trials, and personalized medicine. However, there are several obstacles to implementing AI in this industry, including limited familiarity with the technology, inadequate IT infrastructure, and the difficulty of extracting valuable data from patients' records. One specific application of AI in the pharmaceutical field involves the development of small peptides with antimicrobial properties, which can serve as novel antibiotics to combat superbugs that are resistant to multiple drugs. AI can assist in determining the effectiveness and potency of these peptides, facilitating the development of powerful antibiotics. Despite these challenges, AI holds tremendous potential in the pharmaceutical industry, enabling accelerated innovation, time and cost savings, and ultimately, saving lives. In conclusion, although there are limitations to adopting AI in pharma, there are numerous promising future prospects that could revolutionize the industry and enhance patient outcomes.

KEYWORDS: *Artificial Intelligence, Pharmaceutical, Clinical Trials, Industry, Challenges*

How to cite this paper: Shaikh Sameer Salim | Manoj Kumar "Impact of Artificial Intelligence in the Pharmaceutical World- A Review" Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-7 | Issue-3, June 2023, pp.1113-1118, URL: www.ijtsrd.com/papers/ijtsrd57564.pdf

IJTSRD57564

INTRODUCTION

The pharmaceutical industry has experienced a profound transformation with the integration of Artificial Intelligence (AI), which is extensively applied across various healthcare domains. Due to limited resources and high research costs, many pharmaceutical companies face challenges in discovering and developing new drugs. However, AI technology has emerged as a valuable asset for streamlining drug development processes. Combining human intelligence with computer processing, AI represents an advanced version of computer-aided techniques. It involves gathering information from diverse sources, managing data through rule creation, and leveraging predictive analysis to generate appropriate outcomes and conclusions. Statistical tools, including machine learning and deep learning, are utilized within AI to emulate human behavior, particularly through neural networks. AI techniques play a crucial role in hit series identification, drug molecule formulation, and efficient execution of clinical trials, ultimately driving innovation and facilitating the accurate and rapid production of medicines within the pharmaceutical sector. [1]

Neural networks are computational and mathematical models that establish relationships among given data without prior knowledge of desired outcomes. They produce a range of outcomes that best fit the experimental data while satisfying the given criteria. Artificial Neural Networks (ANNs) are a modified version of neural networks that prove valuable in addressing pharmaceutical research, development, and formulation challenges. Another AI technology, known as fuzzy logic, simplifies complex concepts by mining and presenting information in an easily interpretable format. Users can then devise actions and formulate rules that guide efficient work progress and future prospects.[1], [2]

AI has the potential to revolutionize the pharmaceutical industry in several ways. One significant area is personalized medicine, where AI algorithms can analyze extensive datasets to identify unique patient characteristics that may impact treatment outcomes. This valuable information aids in the development of personalized medicines tailored to individual patients' specific needs. Another way AI enhances drug development is through drug

repurposing, which evaluates existing drugs for new applications based on molecular structure and other characteristics. This approach saves time and resources in the drug development process. [1]

AI also optimizes clinical trials by identifying the most promising patient populations and predicting which patients are likely to respond to treatment. This reduces the time and cost required to bring new drugs to market while ensuring patient safety during trials. Furthermore, AI expedites the drug discovery process by identifying new drug targets and predicting the interactions between different compounds and those targets. This enables researchers to focus their efforts on the most promising drug candidates, saving time and resources. [2]

Role of AI In Drug Development

The process of discovering and developing new drugs is becoming increasingly challenging due to the vast chemical space, making it difficult to find innovative drug molecules. However, the application of artificial intelligence (AI) techniques has proven highly beneficial at various stages of drug development. AI plays a crucial role in identifying and validating drug targets, modeling drugs, and improving their properties. It also assists in designing clinical trials and optimizing decision-making strategies. [3]

One notable AI application is "Open Targets," a strategic program that explores the relationship between drug targets and diseases, guiding the identification of disease-associated targets. Another technique, the 3N-MCTS neural network, outperforms retro synthesis computer-aided systems by devising synthesis routes more efficiently. SPIDER is an AI approach used to determine the role of natural products in drug discovery, while RASAR is an advanced tool that predicts the toxicity of unknown compounds. The DNN system, consisting of interconnected artificial neurons, transforms data and establishes criteria for drug classification based on pharmacological and toxicological information. GANs serve as a foundation for developing next-generation AI techniques. [2]

As of 2023, Machine Learning (ML) is a vital component of AI. It leverages statistical attributes and can be categorized into three types:

Supervised Learning: This approach develops predictive models through regression and classification techniques using input and output data. For example, classifying diseases and predicting drug efficacy and ADME characteristics fall under this category.

Unsupervised Learning: This approach focuses solely on input data and interprets it by clustering and grouping, identifying patterns and features. For instance, clustering data can provide information about disease categories, while feature findings can reveal insights about the origins of disease targets. [3]

Reinforcement Learning: This approach aims to make decisions based on the environment and execute actions to achieve optimal performance. It includes drug design through de novo approaches in the decision-making category, and experimental drug design in the execution category. Modeling and quantum chemistry applications support these processes.

Another subfield of Machine Learning is Deep Learning (DL), which utilizes artificial neural networks to adapt and learn from experimental data. Data mining approaches can be employed to study data, and algorithms can be developed to aid in the discovery of new entities such as genetic markers and novel drug molecules. By harnessing the power of Artificial Intelligence, pharmaceutical product development can address various challenges, leading to reduced drug failures in clinical trials and cost-effective drug design and development. [4]

Tools of AI

UCSF Medical Center has implemented robotic technology to enhance patient safety by preparing and tracking medications. This advanced technology has already successfully prepared more than 350,000 doses of medication with zero errors, surpassing human capabilities in terms of accuracy and efficiency. It is capable of preparing both oral and injectable medications, including complex and hazardous chemotherapy drugs, relieving pharmacists and nurses of this task and allowing them to dedicate more time to patient care.

Additionally, the MEDi Robot was specifically developed to aid in pain management for children by establishing rapport and explaining medical procedures in a child-friendly manner. On the other hand, the Erica robot, originating from Japan, possesses a unique blend of European and Asian facial features and is proficient in speaking Japanese. It can answer questions using human-like facial expressions, enhancing the interaction between humans and robots.

In terms of logistical support, Aethon TUG robots have been designed to autonomously navigate hospital premises, ensuring the efficient delivery of medications, meals, and essential materials throughout the facility.

In the realm of drug discovery, Boston-based biotech company Berg utilizes AI to accelerate the process by identifying and validating disease biomarkers. This

approach significantly reduces costs and eliminates guesswork, ultimately expediting the development of new drugs.[5]

Drug Development Process

The drug development process comprises several steps, including techniques such as High Throughput Screening (HTS) and computational modeling to generate results. It involves two cycles, namely the inductive and deductive cycles, which lead to the identification of hit and lead compounds with desired characteristics. The introduction of automation can minimize errors during this process. The initial step in drug development focuses on identifying novel compounds with desired biological activity. This involves conducting interaction studies with enzymes or organisms to assess their potential. The compound that exhibits biological activity is referred to as a "hit" molecule. Screening libraries of chemical compounds or natural products and utilizing computer simulations help identify these hit molecules. The subsequent step is lead identification, where lead molecules are capable of being developed into the required drug molecule for the targeted disease. Screening assays and animal models are employed to predict the compound's safety and efficacy. Once the lead compound is determined, modifications are made to ensure its safety and effectiveness. [5]

The lead generation phase involves modifying hit molecules to enhance their selectivity and affinity towards the desired target, improve their biological activity, and reduce side effects. Hit expansion is then performed to generate analogues, which are chemical compounds derived from the hit molecules. Medicinal chemists employ a range of reactions to combine these analogues, forming building blocks that contain essential functional groups for interaction with the target's active site.[6]

Artificial Intelligence (AI) can play a crucial role in various aspects of drug development. It can be utilized to identify molecular targets, predict the underlying mechanisms of drug-target interactions, determine hit or lead compounds, synthesize drug-like compounds, repurpose existing drugs, select appropriate populations for clinical trials, study and understand the mode of action of drugs, and design polypharmacology agents. AI has the potential to enhance and expedite multiple stages of the drug development process.[6]

Modulation of size distribution in granules by AI

Computational Intelligence is playing a vital role in drug development by facilitating the creation of optimal particle size distributions during milling processes. The dry granulation method, consisting of compaction and milling steps, is widely used for producing solid dosage forms. To achieve precise control over particle size, researchers are developing various artificial intelligence techniques. These techniques are also employed to investigate the factors and properties of drugs that influence particle size.[4]

Artificial intelligence systems enable the evaluation of the impact of material properties, milling parameters, and conditions on the size distribution of granules. Multiple linear regressions and Artificial Neural Networks (ANN) are utilized to model granule size based on various independent factors. Additionally, Genetic Programming (GP), a model inspired by Darwin's theory of evolution, is employed. GP selects and breeds individuals that can adapt to prevailing conditions and demonstrate fitness.[3]

Through the integration of Computational Intelligence, drug developers can optimize the milling process, achieving precise particle size distributions for enhanced drug formulation.

Role of AI in Clinical Research

The high rate of drug failures in clinical trials and potential issues upon market introduction necessitate the development of a digital platform to address these challenges. While AI holds significant promise, its application in clinical research is still largely theoretical due to the lack of scientific evidence. Nonetheless, AI has a profound impact on clinical research by influencing the success or failure of drug products, reducing development costs, shortening time to market, and minimizing product recalls. It specifically targets three key objectives in clinical research: predicting signals affecting disease pathology, intervention methods, and the impact of time on a patient's condition and quality of life. AI offers numerous advantages over traditional medical practices, such as the ability to analyze pathological patient data, laboratory results, and drug requests to differentiate between normal and abnormal conditions. Neural network frameworks have been effectively employed to interpret results from various diagnostic tests, including MRI, X-ray, and CT scans. AI technology also enables the prediction of allergic reactions and adverse drug events through automated software that aids in reporting and managing such incidents. The integration of mobile phones allows patients to directly input data, enabling more direct engagement during clinical trials. Multiple references corroborate the advantages of AI over traditional medical practices.[7]

The recruitment of suitable patients for clinical trials poses a significant challenge for pharmaceutical companies despite the abundance of patient data

available. The process of identifying and enrolling ideal candidates is time-consuming, leading to average trial durations of 7.5 years and costs ranging from $161 million to $2 billion per drug. Unfortunately, approximately 80 percent of clinical trials fail to meet their deadlines. With over 18,000 ongoing clinical studies recruiting candidates in the US alone, the $65 billion clinical trial market is in need of an overhaul. Extracting valuable data from patient records proves to be a major obstacle for pharmaceutical companies, but AI and machine learning present a solution. [6]

Role of AI in the Design of peptide antibiotics

The development of antibiotic resistance poses a major challenge in finding new antibiotics, raising concerns about their use. Small peptides with antimicrobial properties have emerged as a promising class of antibiotics. However, designing broad-spectrum peptide antibiotics requires detailed knowledge of their chemical characteristics and molecular biology. One approach to creating such peptides involves utilizing peptide array technology to generate two large libraries of 9-amino-acid peptides. The data obtained from this technique, combined with Artificial Neural Networks (ANNs), is used to develop quantitative in silico models for antibiotic activity. Random evaluations of these models have shown promise in predicting the activity of approximately one hundred thousand peptides. Among these peptides, a quarter demonstrated the most potent activity against multidrug-resistant "Superbugs." Consequently, these peptide antibiotics have the potential to effectively treat various superinfections. AI plays a crucial role in the design of novel peptides and assists in determining their efficacy and potency. By incorporating multiple databases on small molecules, peptides, amino acids, and more, AI contributes to the development of targeted and effective drug delivery systems by studying drug-target interactions. Thus, peptide molecules hold significant potential in combating drug resistance and the development of highly effective antibiotics.[8]

Utilizing AI in the Pharmaceutical Industry

The integration of artificial intelligence (AI) into the pharmaceutical industry has the potential to revolutionize innovation by harnessing the power of advanced technologies. AI is a cutting-edge technology that enables computer systems to perform tasks traditionally requiring human intelligence, including decision-making, visual perception, speech recognition, and language translation. In 2011, the healthcare industry was estimated to have a staggering 161 billion GB of data, and AI can effectively analyze and present insights from this vast amount of data, greatly enhancing decision-making processes and leading to significant time, cost, and life-saving benefits.

One prominent application of AI in the pharmaceutical industry is its ability to predict and prevent the occurrence of epidemic outbreaks. By studying historical outbreak data, analyzing social media activity, and leveraging predictive algorithms, AI can accurately forecast the likelihood, location, and timing of potential outbreaks. This information is invaluable for proactive measures, resource allocation, and timely interventions.

AI also facilitates the development of new tools for patients and physicians alike. By leveraging AI technologies, innovative solutions can be created to assist in the diagnosis, treatment planning, and monitoring of patients. Additionally, AI plays a vital role in streamlining and enhancing the research conducted during clinical trials. Predictive analytics can be employed to identify potential trial candidates through analysis of social media data and electronic health records, thereby improving recruitment and participant selection processes.[6]

Limitations

Pharmaceutical companies face several challenges in adopting artificial intelligence (AI) technology. Firstly, there is a sense of unfamiliarity with AI due to its novelty and complex nature, often perceived as a "black box" technology. This lack of understanding hinders its widespread adoption within the industry.

Secondly, the existing IT infrastructure in many pharma companies is not well-equipped to support AI applications. The current systems were not originally designed with AI in mind, necessitating significant investments to upgrade the IT infrastructure to effectively integrate AI capabilities.

Furthermore, a considerable portion of the data available to pharma companies is stored in a free text format. This unstructured data requires additional efforts to collect, organize, and transform it into a format that can be readily analyzed by AI algorithms. The process of collating and preparing the data for analysis can be time-consuming and resource-intensive.

Addressing these challenges requires pharma companies to invest in AI education and training programs, upgrade their IT infrastructure to support AI technologies, and establish robust data management systems to effectively handle unstructured data. Overcoming these hurdles will pave the way for the successful integration of AI into pharmaceutical practices, enabling the industry to

fully harness the transformative potential of this emerging technology.[9]

Future perspectives

The use of artificial intelligence (AI) in the pharmaceutical industry offers various potential benefits and future possibilities. One significant application is the ability to personalize treatment for patients. By analyzing extensive datasets, AI can identify the most effective treatment options tailored to each individual's unique characteristics and medical history.

Another area where AI can contribute is in the development of new tools to support both patients and physicians. These tools, such as digital assistants and chatbots, have the potential to enhance patient outcomes and alleviate the workload of healthcare providers, improving overall healthcare delivery.

Predictive analytics is another valuable aspect of AI in pharma. By leveraging data from social media and doctor visits, AI can identify suitable candidates for clinical trials, expediting the drug development process and enabling faster access to innovative treatments.

AI's role in designing novel drug therapeutics is also noteworthy. For example, AI algorithms can aid in the creation of broad-spectrum antimicrobials to combat the growing challenge of drug resistance, providing new solutions to address this critical issue.

Additionally, AI has proven effective in predicting and managing epidemic outbreaks. By analyzing historical data, monitoring social media activity, and utilizing advanced algorithms, AI can accurately forecast the occurrence, location, and timeline of potential outbreaks, enabling timely intervention and response.

While there are limitations and challenges to overcome in adopting AI in the pharmaceutical industry, the potential benefits and future perspectives are promising. AI has the capacity to revolutionize the industry, improve patient outcomes, and contribute to advancements in drug discovery, personalized medicine, and public health initiatives. [10]

Conclusion

The utilization of artificial intelligence (AI) within the pharmaceutical sector holds great promise, offering the potential for groundbreaking advancements in drug discovery, development, and delivery. While there are challenges to overcome, such as the unfamiliarity with AI technology and the need for proper IT infrastructure, the benefits it brings to the industry are substantial. AI has the capability to identify promising drug targets, optimize clinical trial designs, personalize treatment approaches, and even forecast epidemic outbreaks. The abundance of healthcare data available can be efficiently analyzed by AI systems, providing valuable insights that can save time, resources, and ultimately, lives. To fully harness the potential of AI, the pharmaceutical industry must embrace its integration and actively pursue its application, thereby driving forward healthcare advancements for the betterment of patients worldwide.

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